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research note
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X-TM:Transport Methods Group

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Subject: Release Notification: MILAGRO–1_0_0

Executive Summary

We wish to announce the release 1_0_0 of MILAGRO, the three-dimensional, XYZ Implicit Monte Carlo code for radiative transfer [1]. For this release, we describe the level of verification of the stand-alone MILAGRO package. The MILAGRO verification includes Design by Contract, degenerate test problems, component tests, nightly regression tests, and benchmark verification problems.

1. Introduction

We have had to verify MILAGRO in order to release it. MILAGRO has been verified at several levels. We discuss these verification levels and present results for the benchmark problems.

2. Design by Contract

We use Design by Contract™[1] (DBC) [2] throughout MILAGRO. Both input to and output from functions have to meet requirements. Various levels of DBC exist such that the the degree of checking can be set at compilation time.

3. Degenerate Test Problems

We routinely run simple test problems that, because of their degenerate nature, have analytic solutions.

The first is a steady-state, infinite medium problem. We mock up an XYZ box with reflecting boundary conditions on all sides. Both radiation and material have the same initial temperatures. The box, then, should simply sit there in equilibrium for all time. We will have statistical deviations, of course. A variant of this problem is to replace the reflecting condition on one surface with a vacuum boundary condition and a surface source (isotropic intensity) at the equilibrium temperature. Nominally, the infinite medium problem tests the radiation–material interaction physics and

[1] "Design by Contract" is a trademark of Interactive Software Engineering.

the reflecting boundary condition,

The second is a streaming problem, in which the radiation is decoupled from the material. If a normally incident flux impinges one side of an XYZ box, it should escape the other side in the same direction for a vacuum boundary or reflect to the opposite direction. These streaming problems test the particle tracking, the mesh, and the cell connectivity.

4. **Component/Regression Tests**

Component tests check the correctness of classes. That is, they check that the classes correctly perform the services they were designed to provide. Currently we have component tests for the following classes (or libraries):

1. random number generator
2. mc (Monte Carlo) classes
   (a) coordinate system
   (b) mesh
   (c) layout
3. imc (Implicit Monte Carlo) classes
   (a) opacity
   (b) material state
   (c) particle and particle buffers
   (d) tally

Regression tests are used to track the state of a code by making sure that no unintended changes or side effects occur. Beyond that, our regression tests are also designed to isolate and test certain aspects of the code, such as geometry, mesh, material, streaming, scattering, physical data, computational parameters, random number generators, and parallelism. Thus, our regression tests these lower level aspects at the higher, compile-code level.

Both the component and regression tests are executed nightly using dejagnu, which reports success or failure. A forthcoming note will describe these test in more detail.

5. **Benchmark Problems**

We have run a few one-dimensional (slab) test problems that have analytic solutions. Our results compare well to the analytic solutions. We have reported most of the results in our NECDC98 paper [1], but we present them all here for completeness.

Marshak Wave with Incident Flux.

This Marshak Wave test problem considers a constant, isotropic intensity incident on a slab. The material was purely absorbing with an opacity of $100/T^3$ cm^2/g, a specific heat of 0.1 Jerks/g/keV, and a density of 3.0 g/cm^3. The incident intensity was a Planckian at 1 keV. We modeled the slab as a row of three-dimensional blocks. The y- and z-directions had one cell of thickness 0.01 cm. The x-direction had 200 cells, each of thickness 0.005 cm. The initial temperature for the system was 1e-6 keV. We ran 10,000 particles per timestep, which was a constant 0.001 shake.

The MILAGRO results at 7.4 shakes are shown in Fig. 1. The analytic results were obtained from a fourth order Runge-Kutta code written by Donald Shirk, LANL. The problem was run on the SGI/Cray ASCI Blue machine using 10 processors and full replication. The runtime is unavailable. There was, however, limited parallel speedup. The reason for the poor parallel performance is that we serially construct the mesh and source every cycle, a generality foreshadowing the interfacing to a code with a dynamic mesh. Plus, the number of particles and the timestep were both relatively small, which reduces the fraction of parallelizable work.

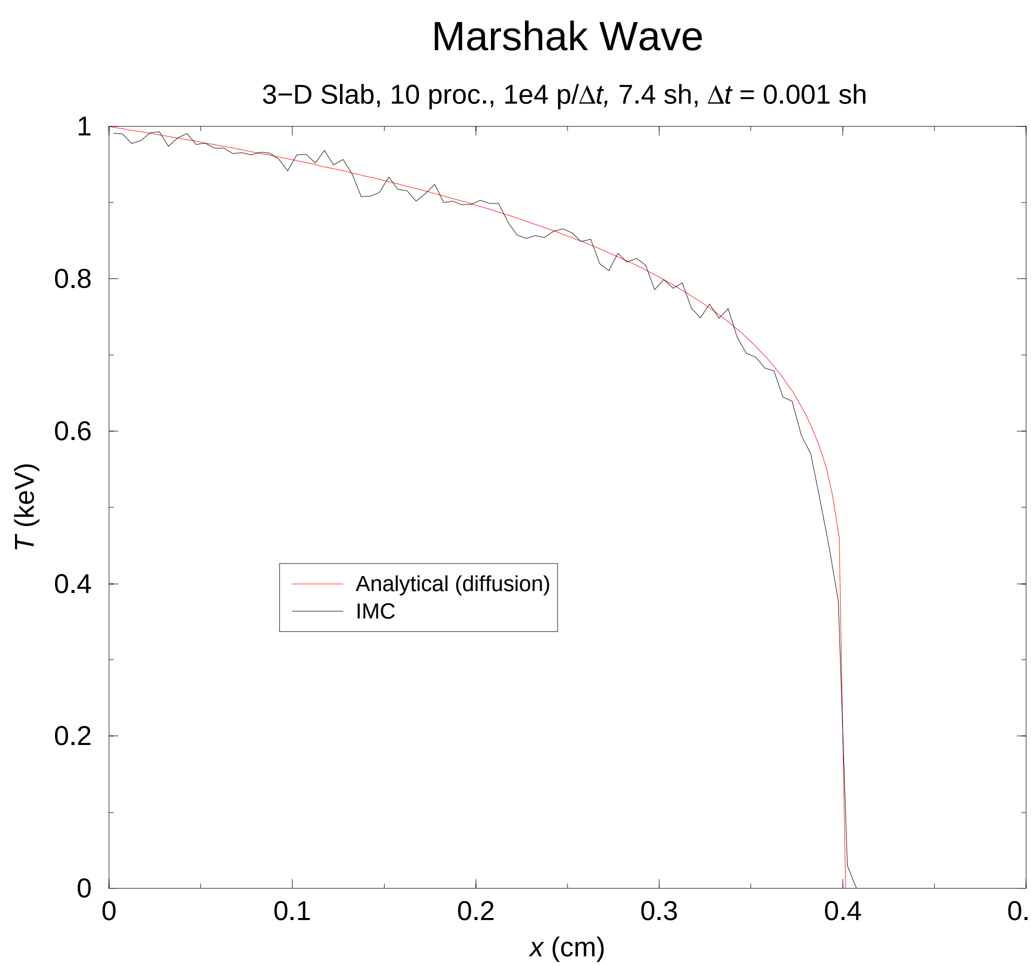

FIG. 1: Marshak Wave with a constant, isotropic incident intensity.

Marshak Wave with Delta Function Source.

The second Marshak Wave variant is again in slab geometry, but with a delta function source of 0.01 Jerks at $x = 0$ cm and $t = 0$ shakes. Although testing the ability to model a delta function may be important, we did not feel it was relevant to verifying our code. So, we ran the problem from $t = 0.1$ shake using the analytic solution as our initial condition. The analytical data used to compare output and to produce the source was produced by Mark Gray's Analytical Test Suite[2]. The slab material had an opacity of $1/T^3$ cm^2/g, a specific heat of 0.1 Jerks/g/keV, and a density of 3.0 g/cm^3.

We modeled the slab with two cells in each of the transverse directions and 40 in the x-direction. The cell size in the x-direction was 0.0025 cm. The cell size was supposed to be 0.0025 in the transverse directions as well, but we accidentally made it ten times larger. This mistake actually made the code run faster, since there were fewer reflections. All boundaries were reflecting. We used 10,000 particles per timestep, which was a constant 0.01 shake. The initial temperatures in non-active cells were 1×10^{-5} keV. We present the results in Fig. 2, where each IMC data point is the average of the four cell values at that x location. The run-time was approximately 4.1 hours on an SGI Octane workstation.

Su and Olson Non-Equilibrium Benchmark.

Su and Olson [3] have a non-equilibrium benchmark. It is a cold, infinite, homogeneous slab with a finite radiation source that exists for a finite amount of time. Of the purely absorbing case and the 50% scattering case, we only present results for the latter so as to demonstrate isotropic scattering in MILAGRO. Regardless, MILAGRO showed excellent agreement in both.

The analytic problem is scaled to a reference temperature, so some trial and error was required to find appropriate physical regimes. Somewhat surprisingly, for unit density and unit opacity, suitable initial temperatures were around 1 keV. Equalizing the initial radiation and material energies resulted in an initial radiation temperature of 1.41 keV and an initial material temperature of 1.00 keV. The specific heat varies with T_{mat}^3 and, for our particular initial conditions, was initially 0.05488 Jerks/g/keV. A suitable timestep was $0.0000\bar{3}$. We used 200 cells in the x-direction, each of thickness 0.1 cm, with reflecting boundary conditions at $x = 0$. The isotropic radiation source, normalized to unity, is located in the region $0 < x < 0.5$ cm and runs from time 0 to $0.0\bar{3}$ shakes. Since the energy in the problem increases while the source is on, we begin the problem with 5000 particles per timestep and linearly ramp up to 50,000 particles at $t = 0.\bar{3}$, or, equivalently, $ct = 100$, where $c = 300$ cm/sh. In order to compare to published results, our results had to be scaled. We multiplied the material energy by 375 and the radiation energy by four times that. The radiation and material energy plots are shown in Figs. 3 and 4, respectively. Note the spikes in the low material energy regions; they are probably noise due to our statistical comb. Note also that the analytic solution has too few data points in some regions.

[2] The Analytical Test Suite is an XTM application used to verify radiation transport packages.

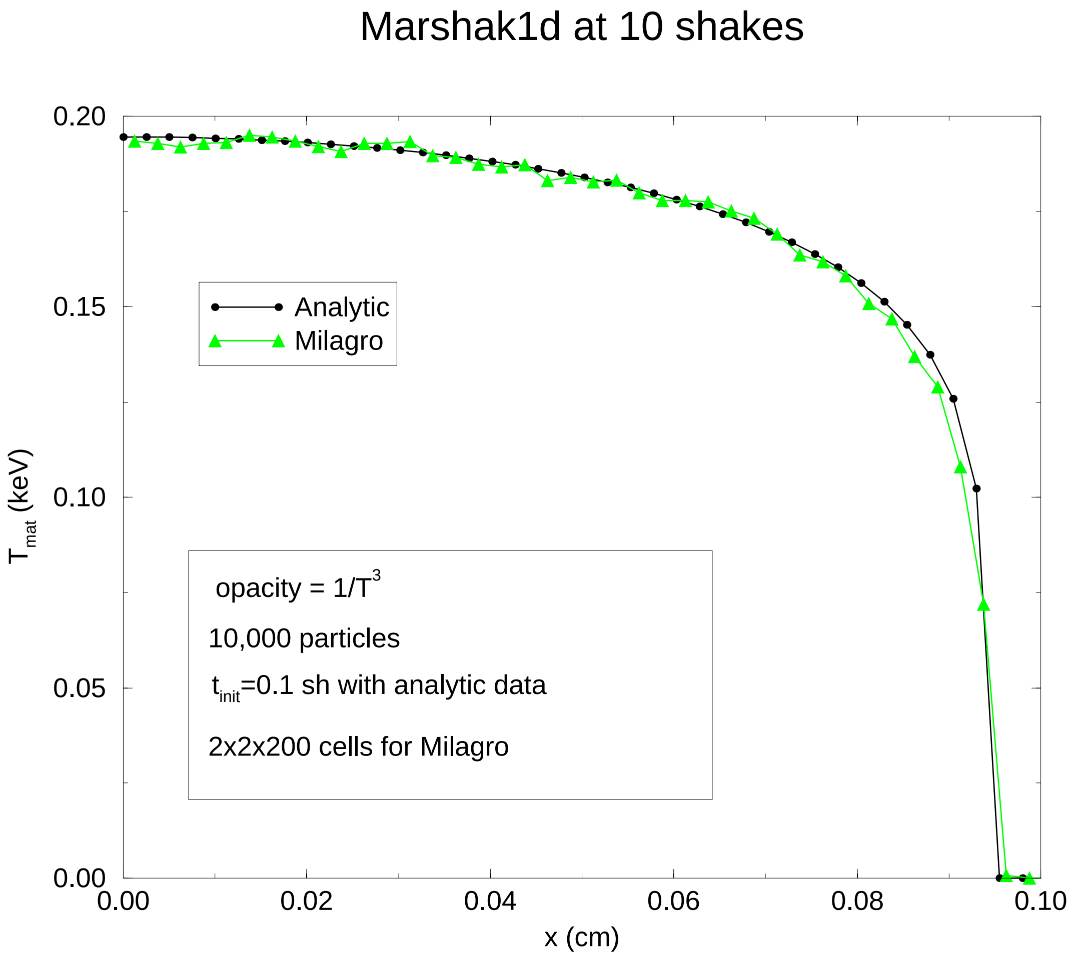

FIG. 2: Marshak Wave with delta function source of 0.01 Jerks at time = 0 and $x = 0$.

Olson Wave

Olson, Auer, and Hall introduce a variant of the Marshak Wave and present solutions from several different methods. We compare our MILAGRO results to their "best" solution, which came from a Variable Eddington Factor (VEF) method that iterated on the time-implicit opacities. We mocked up the problem along the x-direction with Δx=0.01 cm and one 10 cm-thick cell in each of the transverse directions. We used a timestep of 0.01 ct cm, which relates to $1/3 \times 10^{-4}$ sh. The initial number of particles was 1000, and it ramped up at a rate of 10^5 particles/sh with a ceiling of 30,000. The material had a density of 0.38214 g/cm^3, an absorption/emission coefficient of $2.61684/T^3$, a specific heat of 0.14361 jks/g/cm^3, and an initial temperature of 0.056234 keV. Figure 5 shows the material and radiation temperatures from MILAGRO and the VEF method for times of 1, 3, 10, 30, and 100ct cm. The agreement is good. Differences in the wavefronts are probably due to the fact that MILAGRO uses time-explicit opacities.

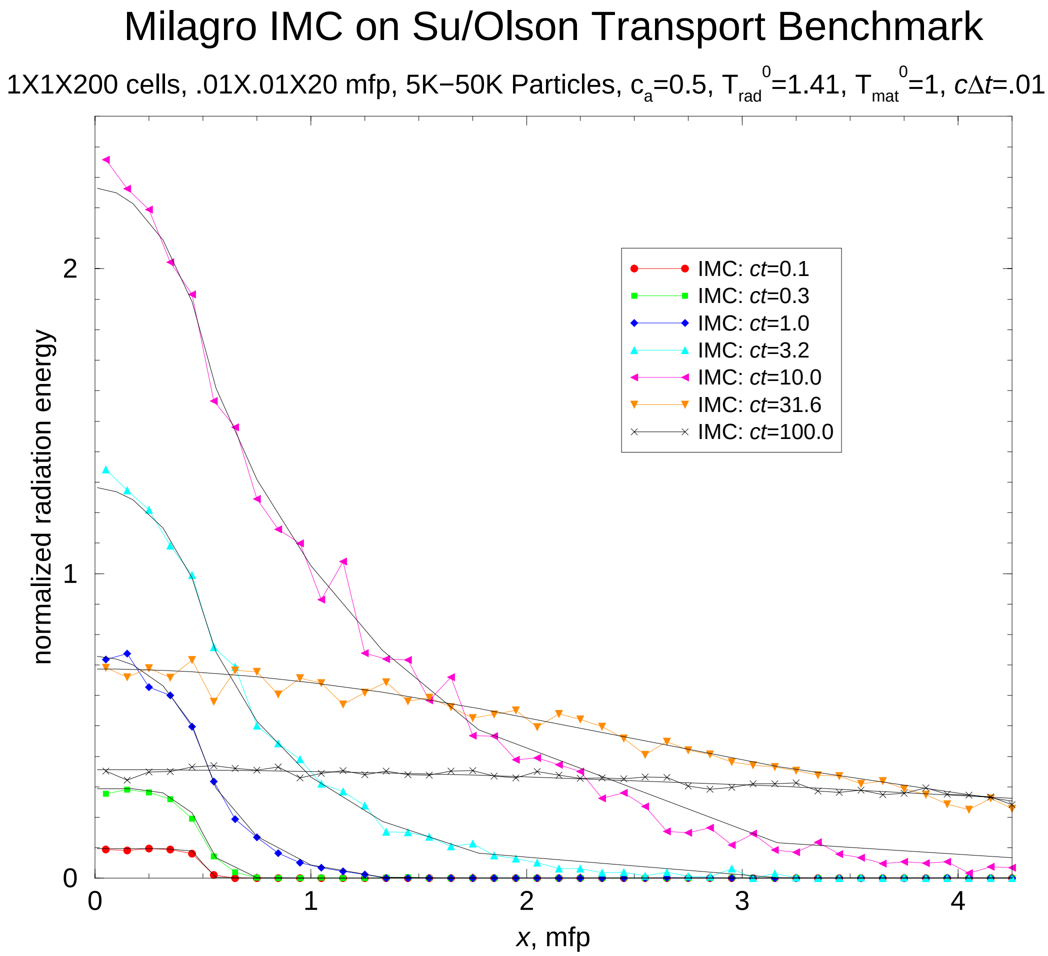

FIG. 3: Normalized radiation energy for Su/Olson non-equilibrium transport benchmark.

References

[1] T. M. Evans and T. J. Urbatsch, "MILAGRO: A parallel Implicit Monte Carlo code for 3-d radiative transfer (U)," in *Proceedings of the Nuclear Explosives Code Development Conference*, (Las Vegas, NV), Oct. 1998. LA-UR-98–4722.

[2] B. Meyer, *Object-Oriented Sofware Construction*. Upper Saddle River, NJ: Prentice Hall, second ed., 1997.

[3] B. Su and G. L. Olson, "An analytical benchmark for non-equilibrium radiative transfer in an isotropically scattering medium," *Annals of Nuclear Energy*, vol. 24, no. 13, pp. 1035–1055, 1997.

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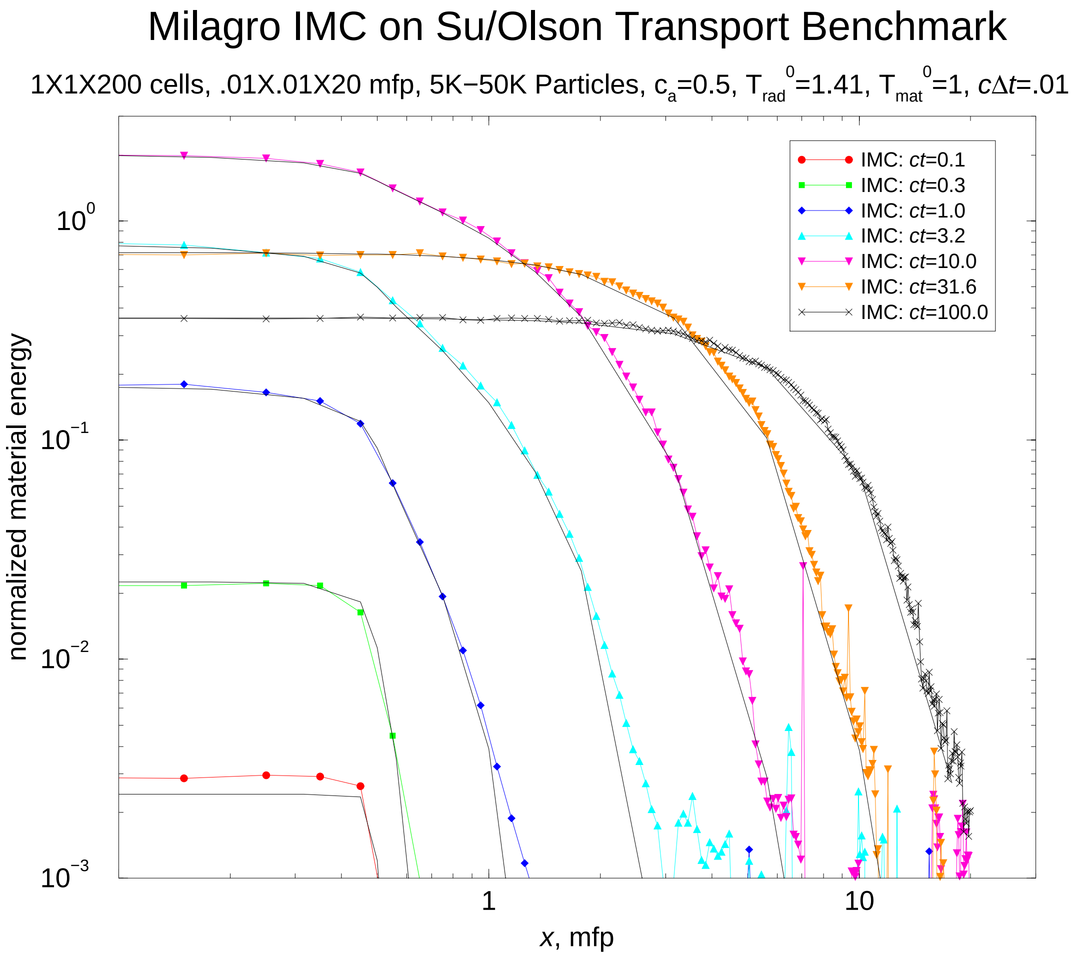

FIG. 4: Normalized material energy for Su/Olson non-equilibrium transport benchmark.

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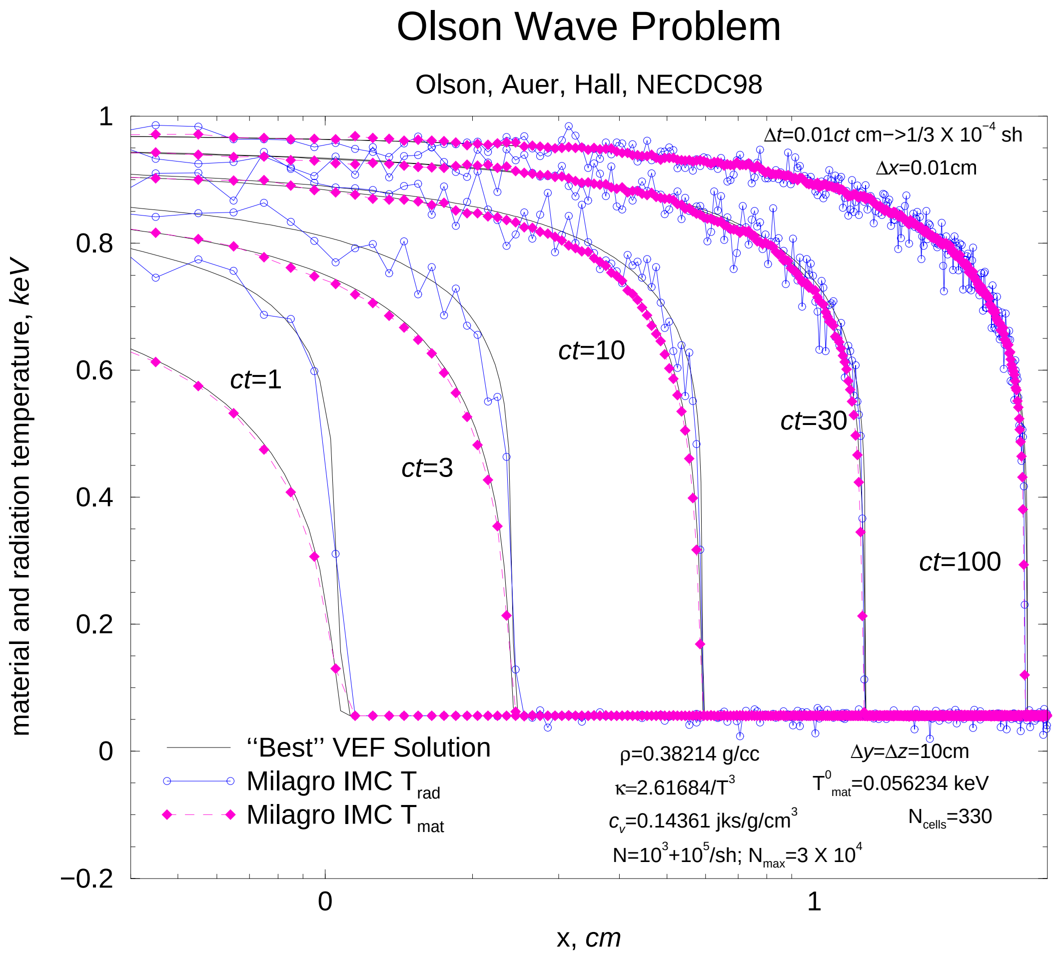

FIG. 5: Radiation and material temperatures from MILAGRO and a VEF method for the Olson Wave.

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